

## Some properties of WKB series

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**Abstract.** We investigate some properties of the WKB series for arbitrary analytic potentials and then specifically for potentials  $x^N$  ( $N$  even), where more explicit formulae for the WKB terms are derived. Our main new results are: (i) We find the explicit functional form for the general WKB terms  $\sigma'_k$ , where one has only to solve a general recursion relation for the rational coefficients. (ii) We give a systematic algorithm for a dramatic simplification of the integrated WKB terms  $\oint \sigma'_k dx$  that enter the energy eigenvalue equation. (iii) We derive almost explicit formulae for the WKB terms for the energy eigenvalues of the homogeneous power law potentials  $V(x) = x^N$ , where  $N$  is even. In particular, we obtain effective algorithms to compute and reduce the terms of these series.

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# 1 Introduction

Semiclassical approximations of the solutions to the wide variety of wave equations in mathematical physics are well known since at least the nineteenth century, mainly based on the ideas of short wavelength approximations. Their applications became of extreme importance in solving the energy eigenvalue problem of the stationary Schrödinger equation. In fact, this has been done by the famous EBK quantization, initiated by Bohr and Sommerfeld for the separable potentials, generalized by Einstein to the integrable potentials (by quantizing the classical invariant tori), and completed by Maslov (by taking into account the phase corrections at the classical turning points and caustics in more than one degree of freedom). This is known under the name torus quantization. Einstein's work was in fact completed in 1917 even before the quantum mechanics was discovered, and it has been later realized that it is (after Maslov phase corrections are taken into account) precisely the leading order semiclassical approximation to the exact solution. Einstein knew from the communications with Henri Poincaré that the integrability in classical Hamiltonian systems is exceptional, and thus that nonintegrability and nonexistence of invariant tori is the generic rule. How to proceed in such case was a mystery for him. It is later through the works of Gutzwiller around 1970 (see his book Gutzwiller 1990) that we got an answer to this question, which is a systematic approach to represent the leading semiclassical approximation as a sum over contributions associated with classical periodic orbits, the so called Gutzwiller theory. All these findings were of crucial heuristic, qualitative and to large extent also quantitative value and importance especially in the course of studying the quantum chaos, which is the study of the quantum signatures of classical chaos.

On the other hand in 1-dim systems more can be done and indeed there is a quite well developed theory (see e.g. Delabaere *et al* (1997), Balian *et al* (1979), Voros (1983) and references therein). Nevertheless if we ask for explicit results not so much is known. However there are the systematic semiclassical procedures in the one dimensional potentials, which are of course always integrable, and where the leading torus approximation is only precisely the first term in a certain WKB series expansion, where each term can be obtained recursively, in principle, and where in certain cases the series can be summed and it can be shown to yield precisely the exact result. In this regard a very important classic and historic paper is by Bender *et al* (1977). See also (Robnik and Salasnich 1997a,b) and Romanovski and Robnik (1999) and (Salasnich and Sattin 1997). The Schrödinger eigenvalue problem is very difficult even for general one dimensional potentials and any analytically tractable WKB approximations and exact results are of extreme importance in qualitative and quantitative understanding of general solutions. Also, they provide a basis for

the many dimensional integrable cases, where almost nothing is known beyond the leading Einstein-Maslov term. In the following we shall use the terminology "WKB series expansion" as the synonym of the "semiclassical expansions" which we clearly define below.

Although at present the WKB theory is very deeply developed and its methods are very important for many applications, there are only a few works where the problem of effective calculation of the terms of WKB expansions is discussed. In this direction a pioneering paper is by Bender *et al* (1977), where the authors investigated the structure of the terms of WKB expansions and also applied the methods to compute the eigenvalues of the potential  $V(x) = x^N$  ( $N$  even). In our present paper we perform further study of the problem of effective computation of WKB series started in Bender *et al* (1977). We obtain new recurrence formulae for WKB terms for arbitrary analytic potentials and for the polynomial potential  $V(x) = x^N$ . The known algorithms are very laborious, because they involve operations of differentiation and collection of similar terms in polynomials, which are extremely time-consuming as the order increases, even when modern computer algebra systems are used. In contradiction, in computing by means of our recurrence formulae one does only arithmetic operations with rational numbers, as we have explicit formulae for the WKB terms, except for the numerical coefficients.

Using the obtained functional form for the general WKB terms  $\sigma'_k$  we give a systematic algorithm for a dramatic simplification of the integrated WKB terms  $\oint \sigma'_k dx$  that enter the energy eigenvalue equation, by showing systematically that the idea of Bender *et al* (1977) can be fully implemented resulting in the maximum possible simplification of the integrated terms. This is achieved by finding terms of the integrand which are complete derivatives of some function and thus give zero contribution when integrated round a closed integration contour in the complexified coordinate plane  $x$ . We also derive almost explicit formulae for the WKB terms for the energy eigenvalues of the homogeneous power law potentials  $V(x) = x^N$ , where  $N$  is even.

These results go substantially beyond the results of Bender *et al* (1977) and indeed it should be emphasized that the main algebraic ideas behind our present work are due to certain remarkable similarities between our present problems and those involved in calculating the normal forms and Lyapunov focus quantities in the power law differential equations (of one degree of freedom) and maps (see Romanovski 1993, Romanovski and Rauh 1998). There are also some common features between the problem of reduction of the coefficients  $\sigma'_k$  of the WKB series and the problem of finding a basis of the ideal of Lyapunov focus quantities (the so-called local 16th Hilbert problem, see Romanovski 1996). Some introduction to the WKB method

can be found in (Bender and Orszag 1978).

We consider the two-turning point eigenvalue problem for the one-dimensional Schrödinger equation

$$[-\hbar^2 \frac{d^2}{dx^2} + V(x)]\psi(x) = E\psi(x). \quad (1)$$

We can always write the wavefunction as

$$\psi(x) = \exp \left\{ \frac{1}{\hbar} \sigma(x) \right\} \quad (2)$$

where the phase  $\sigma(x)$  is a complex function that satisfies the differential equation

$$\sigma'^2(x) + \hbar \sigma''(x) = (V(x) - E) \stackrel{def}{=} Q(x). \quad (3)$$

The WKB expansion for the phase is

$$\sigma(x) = \sum_{k=0}^{\infty} \hbar^k \sigma_k(x). \quad (4)$$

Substituting (4) into (3) and comparing like powers of  $\hbar$  gives the recursion relation

$$\sigma_0'^2 = Q(x), \quad \sigma_n' = -\frac{1}{2\sigma_0'} \left( \sum_{k=1}^{n-1} \sigma_k' \sigma_{n-k}' + \sigma_{n-1}'' \right). \quad (5)$$

Computing few first functions  $\sigma_k'$  by means of the recurrent formula we get

$$\sigma_0' = -\sqrt{Q(x)}, \quad \sigma_1' = \frac{-Q'(x)}{4Q(x)}, \quad (6)$$

$$\sigma_2' = \frac{5Q'(x)^2 - 4Q(x)Q''(x)}{32Q(x)^{\frac{5}{2}}}, \quad (7)$$

$$\sigma_3' = \frac{-15Q'(x)^3 + 18Q(x)Q'(x)Q''(x) - 4Q(x)^2Q^{(3)}(x)}{64Q(x)^4} \quad (8)$$

and

$$\sigma_4' = (1105Q'(x)^4 - 1768Q(x)Q'(x)^2Q''(x) + 448Q(x)^2Q'(x)Q^{(3)}(x) + 304Q(x)^2Q''(x)^2 - 64Q(x)^3Q^{(4)}(x))/2048Q(x)^{\frac{11}{2}}. \quad (9)$$

For the analytical potential  $V(x)$  the following quantization condition is known (see Dunham (1932), Fröman and Fröman (1977), Fedoryuk (1983)):

$$\frac{1}{2i} \oint_{\gamma} \sum_{k=0}^{\infty} \hbar^k \sigma'_k(x) dx = \pi n_q \hbar, \quad (10)$$

where  $n_q \geq 0$  is an integer number and  $\gamma$  is a contour surrounding the turning points on the real axis. This relation is an equation with respect to  $E$  and using it one can find the asymptotic of the eigenvalues  $E_n(\hbar)$  (see e.g. Balian *et al* (1979), Fedoryuk (1983) and references therein). In some cases the series (10) can be summed exactly (see Bender *et al* (1977), Robnik and Salasnich (1997a,b), Romanovski and Robnik (1999), Salasnich and Sattin (1997)).

The zero-order term of the WKB expansion is given by

$$\frac{1}{2i} \oint_{\gamma} d\sigma_0 = \int dx \sqrt{E - V(x)}, \quad (11)$$

the first odd term is

$$\frac{\hbar}{2i} \oint_{\gamma} d\sigma_1 = -\frac{\pi \hbar}{2} \quad (12)$$

and to find the higher order terms we need to compute the functions  $\sigma'_k$  using the recursion relation (5). We note that the odd-order terms (except the first order for  $\sigma'_1$ ) yield integrals that vanish exactly, because, as it follows from the results of Fröman (1966), the functions  $\sigma'_{2k+1}$  are total derivatives.

## 2 An algorithm for computing $\sigma'_k$

We will look for a general formula for the functions  $\sigma'_k$ . As it is known one of the most powerful tools for investigation of recurrence relations is the method of generating functions (see e.g. Graham *et al* 1994). The most widely used in combinatorics generating functions are the ones with a single variable, for example, a generating function for the sequence  $\{g_0, g_1, g_2, \dots\}$  is the formal series

$$G(z) = \sum_{n \geq 0} g_n z^n. \quad (13)$$

For a multi-index sequence  $\{g_{(y_1, \dots, y_m)}\}_{y_i \in \mathbf{N}}$ , where  $\mathbf{N}$  is the set of non-negative integers, a generating function has the form

$$G(z_1, \dots, z_m) = \sum_{y_i \geq 0} g_{(y_1, \dots, y_m)} z_1^{y_1} \dots z_m^{y_m}. \quad (14)$$

Moreover, we can also consider a sequence, where every term has only finite number of indices, but the total number of indices is unbounded (e.g.  $g_{(y_1)}, g_{(y_1, y_2)}, g_{(y_1, y_3, \dots, y_n)}, \dots$ ) with the generating function

$$G(z_1, z_2, \dots) = \sum_{\gamma \in M} g_\gamma \bar{z}^\gamma, \quad (15)$$

where  $M = \cup_{k=1}^{\infty} \mathbf{N}^k$ ,  $\bar{z} = (z_1, \dots, z_s)$  and  $\bar{z}^\gamma = z_1^{\gamma_1} \dots z_s^{\gamma_s}$ . Thus in the last case  $G(z_1, z_2, \dots)$  is an element of the ring of formal power series in the infinite number of variables,  $z_1, z_2, \dots$ .

We now apply the method of generating functions to computing of the WKB expansion for the phase. With any vector  $\nu = (\nu_1, \nu_2, \dots, \nu_l)$  we associate the operator

$$L(\nu) = 1 \cdot \nu_1 + 2 \cdot \nu_2 + \dots + l \cdot \nu_l, \quad (16)$$

where the vector  $\nu$  runs through whole  $M$ .

We will show that the functions  $\sigma'_m$  are of the form

$$\sigma'_m = \sum_{\nu: L(\nu)=m} \frac{U_\nu Q^{m-|\nu|} Q^{(\nu)}}{Q^{\frac{3m-1}{2}}}, \quad (17)$$

where for a vector  $\nu = (\nu_1, \dots, \nu_l)$  we denote  $Q^{(\nu)} = (Q')^{\nu_1} (Q'')^{\nu_2} \dots (Q^{(l)})^{\nu_l}$ ,  $|\nu| = \nu_1 + \dots + \nu_l$  and the coefficients  $U_\nu$  satisfy the recurrence relation

$$U_\nu = \frac{1}{2} \sum_{\mu, \theta \neq 0, \mu + \theta = \nu} U_\mu U_\theta + \frac{(4 - L(\nu) - 2|\nu|) U_{(\nu_1-1, \nu_2, \dots, \nu_l)}}{4} + \sum_{i=1}^{l-1} \frac{(\nu_i + 1) U_{\nu(i)}}{2}, \quad (18)$$

where  $U_0 = -1$  and we put  $U_\gamma = 0$  if among the coordinates of the vector  $\gamma$  there is negative one, and we denote by  $\nu(i)$  ( $i = 1, \dots, l-1$ ) the vector  $(\nu_1, \dots, \nu_i + 1, \nu_{i+1} - 1, \dots, \nu_l)$ .

It should be mentioned that the complexity of functions  $\sigma'_n$  increases rapidly with the order  $n$ , and it is remarkable that applying our almost explicit formulae (17), (18) we can go much further than by using the well-known recursion relation (5) (see the Appendix).

Note that the number of solutions  $\nu$  of the equation

$$L(\nu) = m, \quad (19)$$

where  $m > 0$  and  $\nu$  is a vector with non-negative coordinates, equals the number of partitions  $p(m)$  of the integer  $m$  (there exists a theory and a formula for  $p(m)$ ;

see e.g. Andrews (1976)). Therefore as a corollary of formula (17) we find that the number of terms of the function  $\sigma'_k$  cannot exceed  $p(m)$ . This fact was for the first time observed by Bender *et al* (1977).

We prove the formulae (17), (18) by induction on  $m$ . Indeed, for  $m = 1, 2$  the statement holds. Let us suppose that it is true for all  $m$  less than  $k$ . Then for  $m = k$  we get

$$\frac{\sigma'_i \sigma'_{k-i}}{2\sigma'_0} = \sum_{\theta, \mu: L(\theta)=i, L(\mu)=k-i} -\frac{U_\theta U_\mu Q^{k-|\mu|-|\theta|} Q^{(\mu+\theta)}}{2Q^{\frac{3k-1}{2}}}. \quad (20)$$

Obviously,

$$L(\theta) = i, L(\mu) = k - i \Rightarrow L(\theta + \mu) = k, \quad (21)$$

and here we assume that the dimensions of vectors  $\theta$  and  $\mu$  are the same, if not we simply extend the dimension of the smaller one by putting zeros for the excess coordinates. On the other hand, taking into account that all coefficients of the operator (16) are positive, it is easy to verify that

$$L(\theta + \mu) = k \Rightarrow L(\theta) = j, L(\mu) = k - j, \quad 0 \leq j \leq k \quad (22)$$

(this property is the crucial one for the presented method). Thus (20)–(22) yield

$$\sum_{i=1}^{k-1} \frac{\sigma'_i \sigma'_{k-i}}{2\sigma'_0} = \sum_{\theta, \mu: L(\theta+\mu)=k} -\frac{U_\theta U_\mu Q^{k-|\mu|-|\theta|} Q^{(\mu+\theta)}}{2Q^{\frac{3k-1}{2}}}, \quad (23)$$

i.e. we get an expression of the form (17).

For the last term of the recurrence formula (5) we get

$$\frac{\sigma''_{k-1}}{2\sigma'_0} = \sum_{\mu: L(\mu)=k-1} -U_\mu \left[ \frac{(2 - k - 2|\mu|) Q^{k-|\mu|-1} Q^{(\mu_1+1, \mu_2, \dots, \mu_{k-1})}}{4Q^{\frac{3k-1}{2}}} + \frac{Q^{k-|\mu|-1} (Q^{(\mu)})'}{2Q^{\frac{3k-3}{2}}} \right] \quad (24)$$

Note that for the vector  $\mu = (\mu_1, \dots, \mu_{k-1}, 0)$

$$[Q^{(\mu)}]' = \sum_{i=1}^{k-1} \mu_i Q^{(\hat{\mu}(i))}, \quad (25)$$

where we denote by  $\hat{\mu}(i)$  ( $i = 1, \dots, k-1$ ) the vector  $(\mu_1, \dots, \mu_i - 1, \mu_{i+1} + 1, \dots, \mu_k)$  ( $i = 1, \dots, k-1$ ). It is readily seen that  $L(\hat{\mu}(i)) = L(\mu) + 1 = k$ , therefore, formulae (5), (23)–(25) yield that (17), (18) hold.  $\square$

Using the recurrence relation (18) we can obtain the differential equation for the generating function of the sequence  $U_\nu$

$$U(\bar{z}) = U(z_1, \dots) = \sum_{\nu \in M} U_\nu \bar{z}^\nu. \quad (26)$$

Let us rewrite (18) in the form

$$\begin{aligned} U_{(\nu_1, \dots, \nu_l)} = & \frac{1}{2} \sum_{\mu, \theta \neq 0, \mu + \theta = \nu} U_\mu U_\theta + U_{(\nu_1-1, \nu_2, \dots, \nu_l)} - \frac{3}{4} \nu_1 U_{(\nu_1-1, \nu_2, \dots, \nu_l)} - \\ & \frac{1}{4} \sum_{i=2}^l (i+2) \nu_i U_{(\nu_1-1, \nu_2, \dots, \nu_l)} + \sum_{i=1}^{l-1} \frac{(\nu_i + 1) U_{\nu(i)}}{2} - [\nu = 0], \end{aligned} \quad (27)$$

where  $[\alpha = \beta]$  denotes the function, which equals 1 if  $\alpha = \beta$  and 0 otherwise.

Using obvious properties of generating functions (see e.g. Graham *et al* 1994) we get from (27)

$$U = \frac{1}{2}(U+1)^2 + z_1 U - \frac{3}{4} z_1 (z_1 U)'_{z_1} - \sum_{i=2}^l \frac{i+2}{4} z_1 z_i U'_{z_i} + \frac{1}{2} \sum_{i=1}^{l-1} z_{i+1} U'_{z_i} - 1. \quad (28)$$

It means if we fix any integer  $l$  and, therefore, the variables  $z_1, \dots, z_l$ , then the function

$$\hat{U}(z_1, \dots, z_l) = U(z_1, \dots, z_l, 0, 0, \dots) \quad (29)$$

is the solution of the equation (28) with the initial conditions

$$\hat{U}(0) = -1, \hat{U}'_{z_i}(0) = -\frac{1}{2^{i+1}} \quad (30)$$

(we get the initial conditions from (18) taking into account that  $U_{(0, \dots, 0, 1)} = -\frac{1}{2^{i+1}}$  for the vectors with the only  $i$ th coordinate different from zero). So, the coefficients  $U_\nu$  that enter the functions  $\sigma'_k$  (17) are precisely the coefficients of the Taylor expansion of the function  $\hat{U}$  defined by the differential equation (28) with the initial conditions (30).

Coefficients of the form  $U_{(n, 0, \dots, 0)}$  depend on the coefficients of the same form. Therefore we get from (28) that the function  $U(z) = \sum_{n=0}^{\infty} U_n z^n$  satisfies the differential equation

$$U = \frac{1}{2}(U+1)^2 + zU - \frac{3}{4} z(zU)'_z - 1, \quad (31)$$

which is the Riccati equation

$$3z^2 U'_z - 2U^2 - zU + 2 = 0. \quad (32)$$



Note that as an immediate corollary of formula (17) we get that for the harmonic oscillator, i.e. when  $Q = x^2 - E$ , the WKB series (10) terminates after the first two terms, namely,

$$\oint_{\gamma} d\sigma_k = 0 \quad (33)$$

for all  $k \geq 2$ . Indeed, in this case (17) yields

$$\sigma'_m = \sum_{i=0}^{[m/2]} \frac{U_{(m-2i,i)} 2^{m-i} x^{m-2i}}{\sqrt{x^2 - E}^{3m-1-2i}}, \quad (34)$$

where  $[m/2]$  stands for the integer part of  $m/2$ .

It is obvious

$$\text{Res}_{\infty} \frac{x^{m-2i}}{\sqrt{x^2 - E}^{3m-1-2i}} = 0 \quad (35)$$

for all  $m > 1$ . Therefore (33) takes place.

### 3 An algorithm for the simplification of the functions $d\sigma_k$

It was pointed out by Bender *et al* (1977) that the functions  $d\sigma_k$  can be dramatically simplified by adding and subtracting total derivatives (obviously, such operation does not change the integrals (10)). They also carried out numerical experiments to obtain different simplifications of these functions. It is easily seen that the formula (17) provides an effective way to reduce the number of terms in the expressions for the functions  $d\sigma_k$ .

We will look for a function of the form

$$P_k = \sum_{\mu: L(\mu)=k} \frac{W_{\mu} Q^{k-|\mu|} Q^{(\mu)}}{Q^{\frac{3k}{2}}}, \quad (36)$$

where  $W_{\mu}$  are to be determined, such that

$$\frac{d}{dx} P_k = \sigma'_{k+1} \quad (37)$$

By comparing coefficients of  $\frac{Q^{k+1-|\nu|} Q^{(\nu)}}{Q^{\frac{3k+2}{2}}}$ , in both parts of (37) we get the system

$$\frac{3 - L(\nu) - 2|\nu|}{2} W_{(\nu_1-1, \nu_2, \dots, \nu_l)} + \sum_{i=1}^{l-1} (\nu_i + 1) W_{\nu(i)} = U_{\nu}, \quad (38)$$

where  $\nu = (\nu_1, \dots, \nu_l)$  runs through the whole set of solutions of equation (19) and  $U_\nu$  are defined by the recurrence relation (17),(18).

Thus to simplify the function  $\sigma'_{k+1}$  one can solve the system (38) of  $p(k+1)$  equations in  $p(k)$  variables  $W_\mu$ . For example, to simplify  $\sigma'_4$  we write down the corresponding system (38) and get

$$\begin{aligned} U_4 &= -\frac{9}{2}W_3 \\ U_{(2,1)} &= 3W_3 - \frac{7}{2}W_{(1,1)} \\ U_{(1,0,1)} &= W_{(1,1)} - \frac{5}{2}W_{(0,0,1)} \\ U_{(0,2)} &= W_{(1,1)} \\ U_{(0,0,0,1)} &= W_{(0,0,1)} \end{aligned} \quad (39)$$

where  $U_4 = 1105/2048$ ,  $U_{(2,1)} = -1768/2048$ ,  $U_{(0,2)} = 304/2048$ ,  $U_{(1,0,1)} = 448/2048$ ,  $U_{(0,0,0,1)} = -64/2048$ . We see that the matrix, corresponding to the first three equations is the triangular one, so we can kill three terms in the expression for  $d\sigma_4$ . Computing we get

$$W_3 = -\frac{1105}{9216}, W_{(1,1)} = \frac{221}{1536}, W_{(0,0,1)} = -\frac{23}{768}. \quad (40)$$

Hence

$$\sigma'_4 - \frac{d}{dx}P_3 = \frac{7Q''(x)^2 - 2Q(x)Q^{(4)}(x)}{1536Q(x)^{7/2}}, \quad (41)$$

in accordance with Bender *et al* (1977).

Let us denote by  $\tilde{p}(k)$  the number of partitions of  $k$  which contain at least one 1. Obviously,  $p(k) = \tilde{p}(k+1)$ . It appears that the optimal strategy to simplify  $\sigma'_k$  is as follows. In system (38) where  $L(\nu) = k$  we consider the equations with  $\nu$  such that  $\nu_1 \neq 0$ . There are  $\tilde{p}(k) = p(k-1)$  such equations and according to (36) we have exactly  $p(k-1)$  variables. It turns out that we can always write the systems with  $U_\nu$  such that  $\nu_1 \neq 0$  in the triangular form (like system (39)). To see this we set the following order on vectors of  $\mathbf{N}^l$ : we say that  $\nu < \mu$  if the first nonzero entry from the left in  $\mu - \nu$  is positive (this order is known in computational algebra as the lexicographic one). Then if we write down the equations of the system (38), corresponding to  $U_{\nu^{(1)}}, U_{\nu^{(2)}}, \dots$  in the decreasing order  $\nu^{(1)} > \nu^{(2)}, \dots$  and the variables  $W_\mu$  in these equations also in the decreasing order then we get that the matrix corresponding to the first  $p(k-1)$  equations is the triangular  $p(k-1) \times p(k-1)$  matrix (because  $\nu(i) > (\nu_1 - 1, \nu_2, \dots, \nu_l)$  for  $1 \leq i \leq l-1$ ). Moreover, the diagonal elements of the matrix are equal to  $(3 - L(\nu) - 2|\nu|)/2$  and, therefore, are different from zero. Hence, we get that after the simplification  $\sigma'_{2n}$  contains at most  $p(2n) - p(2n-1)$  terms.

To end this section we show that in some cases we can replace calculation of contour integral by computing a Riemann integral, namely we shall show that formula (43) below applies.

First we note that taking into account that  $Q = V(x) - E$  we can write for even  $m$  formula (17) in the form

$$\sigma'_m = \sum_{\nu: L(\nu)=m} \frac{2^{\frac{m}{2}-1+|\nu|} i}{(m-3+2|\nu|)!!} \frac{\partial^{\frac{m}{2}-1+|\nu|}}{\partial E^{\frac{m}{2}-1+|\nu|}} \frac{U_\nu V^{(\nu)}}{\sqrt{E-V}}. \quad (42)$$

Let us now suppose that  $Q = V(x) - E$ , where  $V(x)$  is an analytic function with one minimum and  $V'(x) \neq 0$ , if  $x \neq 0$ . We will show that

$$\oint d\sigma_m = 2 \sum_{\nu: L(\nu)=m} \frac{2^{\frac{m}{2}-1+|\nu|} i}{(m-3+2|\nu|)!!} \frac{\partial^{\frac{m}{2}-1+|\nu|}}{\partial E^{\frac{m}{2}-1+|\nu|}} \int_{x_1}^{x_2} \frac{U_\nu V^{(\nu)}}{\sqrt{E-V}} dx, \quad (43)$$

where  $V(x_1) = V(x_2) = E_0$ ,  $x_1 < x_2$ . Taking into account (42) it is easy to see that to prove (43) it is sufficient to show that

$$\oint_\gamma \frac{\partial^{\frac{m}{2}-1+|\nu|}}{\partial E^{\frac{m}{2}-1+|\nu|}} \frac{V^{(\nu)}}{\sqrt{E-V}} dx = 2 \frac{\partial^{\frac{m}{2}-1+|\nu|}}{\partial E^{\frac{m}{2}-1+|\nu|}} \int_{x_1}^{x_2} \frac{V^{(\nu)}}{\sqrt{E-V}} dx. \quad (44)$$

Note that due to the theorem on differentiation upon a parameter (see e.g. Sidorov *et al* 1976) if

$$F(E) = \oint_\gamma f(x, E) dx \quad (45)$$

and

- 1)  $\gamma$  is a finite piecewise-smooth curve;
- 2) the function  $f(x, E)$  is continuous with respect to  $(x, E)$  for  $x \in \gamma, E \in D$ , where  $D$  is a domain of the complex plane;
- 3) for every fixed  $x \in \gamma$  the function  $f(x, E)$  is analytic upon  $E$  in  $D$ , then  $F(E)$  is analytic in  $D$  and

$$F'(E) = \oint_\gamma \frac{\partial f(x, E)}{\partial E} dx, \quad (46)$$

for  $E \in D$ .

Let us cut the complex plane between the turning points  $x_1$  and  $x_2$  to get a single-valued function and fix the contour  $(x_1 + \rho, x_2 - \rho) \cup c_1 \cup (x_2 - \rho, x_1 + \rho) \cup c_2$ , where  $\rho$  is small  $c_1, c_2$  are circles :  $c_1 = x_2 + \rho e^{it}$ ,  $c_2 = x_1 + \rho e^{it}$  and  $t \in [0, 2\pi]$ . Then the conditions 1)-3) are satisfied (with  $D$  being a small neighborhood of  $E_0$ ). Therefore

$$\oint_\gamma \frac{\partial^{\frac{m}{2}-1+|\nu|}}{\partial E^{\frac{m}{2}-1+|\nu|}} \frac{V^{(\nu)}}{\sqrt{E-V}} dx = \frac{\partial^{\frac{m}{2}-1+|\nu|}}{\partial E^{\frac{m}{2}-1+|\nu|}} \oint_\gamma \frac{V^{(\nu)}}{\sqrt{E-V}} dx = \quad (47)$$

$$\frac{\partial^{\frac{m}{2}-1+|\nu|}}{\partial E^{\frac{m}{2}-1+|\nu|}}(2 \int_{-x_0+\rho}^{x_0-\rho} \frac{V^{(\nu)}}{\sqrt{E-V}} dx + \oint_{c_1} \frac{V^{(\nu)}}{\sqrt{E-V}} dx + \oint_{c_2} \frac{V^{(\nu)}}{\sqrt{E-V}} dx).$$

Let us denote

$$g(E) = \oint_{c_1} \frac{V^{(\nu)}}{\sqrt{E-V}} dx. \quad (48)$$

Due to the theorem mentioned above  $g(E)$  is analytic in a neighborhood of  $E_0$ , therefore

$$g(E) \approx g(E_0) + g'(E_0)(E - E_0). \quad (49)$$

Noting that

$$|g(E_0)| = \left| \oint_{c_1} \frac{V^{(\nu)}}{\sqrt{E_0-V}} dx \right| = \left| \oint_{c_1} \frac{V^{(\nu)}}{\sqrt{V'(x_1)(x-x_1)+\dots}} dx \right| < \text{const } \rho^{1/2} \quad (50)$$

we obtain that  $g(E) \rightarrow 0$  when  $\rho \rightarrow 0, E \rightarrow E_0$ . It means that formula (44) indeed holds. This formula has been found useful for computing the WKB series for Coulomb potential and the potential  $V(x) = U_0/\cos^2(\alpha x)$  (Robnik and Salasnich 1997a,b).

## 4 Potentials of the form $V(x) = x^N$ .

In recent decades many studies have been devoted to the investigation of the semi-classical expansions for the potentials of the form  $V(x) = x^N$  and important results have been achieved (see e.g. Balian *et al* (1979), Voros (1983) and references therein).

One of the basic formulae for these potentials was obtained by Bender *et al* (1977) and is as follows:

$$\pi(n_q + \frac{1}{2}) = E^{1/N+1/2} \sum_{n=0}^{\infty} E^{-n(1+2/N)} a_n(N), \quad (51)$$

where  $N$  is an even integer number,

$$a_n(N) = \frac{(-1)^n 2^{1-n} \sqrt{\pi} \Gamma(1 + \frac{1-2n}{N}) P_n(N)}{(2+2n)! \Gamma(\frac{3-2n}{2} + \frac{1-2n}{N})} \quad (52)$$

and  $P_n(N)$  are polynomials of the variable  $N$  with integer coefficients. The first eight polynomials  $P_n(N)$  were computed using MACSYMA computer algebra program by Bender *et al* (1977) for the general potential  $V(x) = x^N$  and, as it was mentioned, the computation of the eighth polynomial has already faced difficulties. When  $N$

is a fixed integer number then instead of the polynomials  $a_n$  we have integers. The special case of quartic oscillator ( $N = 4$ ) has been deeply investigated by Balian, Parisi, Voros and others. In this case the expression of the type (51) is written (Balian *et al* 1979) in the form

$$2\pi(n_q + \frac{1}{2})\hbar = \sum_{n=0}^{\infty} b_n \sigma^{1-2n} \hbar^{2n}, \quad (53)$$

where

$$\sigma = E^{3/4} B(3/2, 1/4) \quad (54)$$

is the classical action around the closed orbit of energy  $E$  (here  $B(x, y)$  is the beta function) and  $b_n$  in this case are rational numbers. As it is reported by Balian *et al* (1979) with REDUCE language they were able to compute the first seventeen coefficients  $b_n$ . Then they had to switch to the ordinary numerical computation and computed  $b_n$  up to  $n = 53$  (in (Voros 1983) the results of computation up to  $n = 60$  are presented).

It was mentioned in Balian *et al* (1979) and in Bender *et al* (1977) that the authors do not know any closed form or a simple law for the coefficients  $a_n(N)$  and  $b_n$ . In this section we partially answer this question. Although we also were not able to find any closed form for the functions  $a_n$  (or numbers  $b_n$ ) we obtain a simple recurrence formula, where only operations of summation and multiplication of rational numbers are involved, whereas using the usual way of the above mentioned papers one needs first to compute rational functions of the form  $f(x, \sqrt{E - x^N})$  and then evaluate contour integrals. We carried out computer experiments and found out that using our algorithm with Mathematica 4.0 on a PC with 128 MB RAM we were able to compute in closed arithmetic form the coefficients  $b_n$  at least up to  $n = 190$  for the quartic potential (see also the Appendix).

It can be proven (Robnik and Romanovski 2000) by induction using the recursion relation (5) that for the potential  $V(x) = x^N$  the coefficients  $\sigma'_k$  ( $k \geq 1$ ) of the WKB expansion have the form

$$\sigma'_k = -\frac{(-i)^{3k-1} x^{-k+N}}{(E - x^N)^{\frac{3k-1}{2}}} \sum_{j=0}^{k-1} A_{k-j-1,j} E^{k-j-1} x^{jN}, \quad (55)$$

where we choose  $\sqrt{E - x^N} = i\sqrt{x^N - E}$ , and the coefficients  $A_{k-j-1,j}$  of the monomials  $E^{k-j-1} x^{jN}$  are computed according to the recurrence formula

$$A_{s,l} = \frac{1}{2} \sum_{i=0}^s \sum_{j=0}^{l-1} A_{i,j} A_{s-i,l-1-j} + \frac{l(2+N) + (2+3N)s - N}{4} A_{s,l-1} + \frac{(N-1)l + N - s}{2} A_{s-1,l}. \quad (56)$$

with  $A_{0,0} = N/4$  and

$$A_{\alpha,\beta} = 0 \text{ if } \alpha < 0 \text{ or } \beta < 0. \quad (57)$$

Using equation (56) we can get the differential equation for the generating function of the coefficients  $A_{s,l}$ , and in the special case  $A_{s,0}$  one can find the explicit formula (Robnik and Romanovski 2000)

$$A_{s,0} = \frac{N!}{2^{s+2}(N-s-1)!}. \quad (58)$$

For even  $k$ , ( $k \leftrightarrow 2k$ ) we can write formula (55) in the form

$$\sigma'_{2k} = \sum_{j=0}^{2k-1} \frac{i2^{3k}}{(6k-3)!!} A_{2k-j-1,j} E^{2k-j-1} x^{-2k+(j+1)N} \frac{\partial^{3k}}{\partial E^{3k}} (E - x^N)^{1/2}. \quad (59)$$

As above we can replace the integration on a contour with the integration between turning points, then, taking into account that

$$\int_0^a x^{\alpha-1} (a^\theta - x^\theta)^{\beta-1} dx = \frac{a^{\theta(\beta-1)+\alpha}}{\theta} B\left(\frac{\alpha}{\theta}, \beta\right), \quad (60)$$

where  $\alpha, \theta, \operatorname{Re} \alpha, \operatorname{Re} \beta > 0$ , and  $B$  is the beta-function, and noting that

$$\begin{aligned} & \frac{\Gamma(\frac{3}{2} + s + \frac{1-2k}{N} + 1)}{\Gamma(\frac{3}{2} + s + \frac{1-2k}{N} - 3k)} = \\ & \left(\frac{3}{2} + s + \frac{1-2k}{N}\right) \left(\frac{3}{2} + s + \frac{1-2k}{N} - 1\right) \dots \left(\frac{3}{2} + s + \frac{1-2k}{N} - 3k\right) \end{aligned} \quad (61)$$

we get from (59)

$$\oint_{\gamma} d\sigma_{2k} = 2 \int_{-E^{1/n}}^{E^{1/n}} d\sigma_{2k} = \frac{2^{3k+1} i \sqrt{\pi}}{(6k-3)!! N} E^{\frac{1}{2} + \frac{1}{N}} \sum_{s=0}^{2k-1} A_{2k-s-1,s} E^{-\frac{2k}{N}-k} \frac{\Gamma(\frac{1-2k}{N} + s + 1)}{\Gamma(\frac{3}{2} + s + 1 - 3k + \frac{1-2k}{N})}, \quad (62)$$

and using the equality  $\Gamma(1+z) = z\Gamma(z)$  we obtain finally the coefficients of the WKB expansion

$$\begin{aligned} \oint_{\gamma} \sigma'_{2k} dx = & \frac{i2^{3k+1} \sqrt{\pi}}{(6k-3)!! N} E^{\frac{1}{2} + \frac{1}{N} - \frac{2k}{N} - k} \frac{\Gamma(\frac{1-2k}{N} + 1)}{\Gamma(\frac{3-2k}{2} + \frac{1-2k}{N})} (A_{2k-1,0} \prod_{s=1}^{2k-1} (\frac{3-2k}{2} + \\ & \frac{1-2k}{N} - s) + \sum_{i=1}^{2k-1} A_{2k-i-1,i} \prod_{s=1}^i (s + \frac{1-2k}{N}) \prod_{s=1}^{2k-i-1} (\frac{3-2k}{2} + \frac{1-2k}{N} - s)), \end{aligned} \quad (63)$$

where  $k \geq 1$  and  $A_{2k-i-1,i}$  are computed according to (56) and

$$\oint_{\gamma} \sigma'_0 dx = \frac{2iE^{\frac{1}{2} + \frac{1}{N}} \sqrt{\pi} \Gamma(1 + \frac{1}{N})}{\Gamma(\frac{3}{2} + \frac{1}{N})}. \quad (64)$$

## 5 Conclusions

In this paper we have investigated the WKB approximations as a series for arbitrary analytic potentials. Following the classic paper by Bender *et al* (1977) we have achieved the following results: (i) We find the explicit functional form for the general WKB terms  $\sigma'_k$ , where one has only to solve a general recursion relation for the *numerical rational* coefficients. (ii) We give a systematic algorithm for a dramatic simplification of the integrated WKB terms  $\oint \sigma'_k dx$  that enter the energy eigenvalue equation. (iii) We derive almost explicit formulae for the WKB terms for the energy eigenvalues of the homogeneous power law potentials  $V(x) = x^N$ , where  $N$  is even. In particular, we obtain effective algorithms to compute and reduce the terms of these series. In computing by means of these formulae we manipulate only with *numbers* and do not need to collect similar terms of a polynomial, which we must do otherwise when we use just the recursion formula (5). Application of the obtained formulae along with the reduction formula (38) considerably simplifies calculations, especially if we need to compute high order terms.

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## Appendix

Here we present the results of computer experiments which we carried out with Mathematica 4.0 on our PC with 450 MHz processor and 128 MB RAM to compare the efficiency of our algorithms based on equations (17), (18) and (56), (63) with traditional ones.

To compute  $\sigma'_n$  by Mathematica using formula (5) one can just use it in the form presented in the text, but for computing by means of formulae (17), (18) a procedure has to be written.

Table 1: (a) the order  $n$  of the coefficient  $\sigma'_n$ , (b) the number of terms in the coefficient  $\sigma'_n$  (equals  $p(n)$ ), (c) CPU time in seconds for computing  $\sigma'_n$  by means of formula (5), (d) CPU time for computing  $\sigma'_n$  using formulae (17), (18).

(a)	(b)	(c)	(d)	(a)	(b)	(c)	(d)
10	42	0.47	0.54	30	5604	18,542	1,402
15	176	5.7	5.2	34	12310	114,219	4,981
20	627	83	41	35	14883	–	6,733
25	1958	1,509	256	40	37338	–	29,940

In the case of the potential  $V(x) = x^4$  for computing  $\oint \sigma'_{2n} dx$  one can use formulae (56), (63) precisely in the form presented in the paper, but it is necessary preliminary to define  $A_{-1,i} = A_{i,-1} = 0$ .

In (Voros 1983) the table of results of numerical calculations of the numbers

$$A_n = \frac{2^{-\frac{3}{2}-n} \pi b_n \csc(\frac{(3-6n)\pi}{4})}{\Gamma(2n-1)}$$

which should not be confused with our  $A_{s,l}$  and where the numbers  $b_n$  are defined in equation (53), with an estimated accuracy of 34 digits are presented and it is mentioned there that the accuracy is not guaranteed for  $n$  close to 60. Indeed, we found perfect correspondence with the table of (Voros 1983) up to  $n = 52$ , however for larger  $n$  there is a disagreement with our calculations, presented in Table 2 (digits which differ from those obtained by Voros (1983) are underlined). It should be emphasized that here we calculate  $A_n$  in the exact arithmetic form, which includes rational numbers and the gamma function, but show here the numerical results just for the purpose of comparing them with those of (Voros 1983).

We computed the coefficients  $b_n$  in exact arithmetic form according to formulae (56), (63) up to  $n = 190$  and it took 143555 sec CPU time to do so. It was possible to continue computations according to the memory capacity, however the computations became too time consuming. As it is reported by Balian *et al* (1979) with REDUCE language they were able to go up to  $n = 16$ .



Table 2:  $V(x) = x^4$ 

n	$A_n$
53	0.9949789006826957939983352522204 <u>201</u>
54	-0.99507337304487214360383324779308 <u>91</u>
55	0.99516435663454610073093354191234 <u>95</u>
56	-0.99525204117217161254926125130224 <u>71</u>
57	0.995336602869245232422036639479624 <u>0</u>
58	-0.99541820560946123269490593243941 <u>96</u>
59	0.995497002008086630872969891605034 <u>1</u>
60	-0.99557313436395513681995253972048 <u>94</u>

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